

Article

Theoretical and Empirical Characterization of Water as a Factor: Examples and Related Issues with the World Trade Model

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Abstract: This article originates from the theoretical and empirical characterization of factors in the World Trade Model (WTM). It first illustrates the usefulness of this type of model for water research to address policy questions related to virtual water trade, water constraints and water scarcity. It also illustrates the importance of certain key decisions regarding the heterogeneity of water and its relation to the technologies being employed and the prices obtained. With regard to WTM, the global economic input–output model in which multiple technologies can produce a “homo-geneous output”, it was recently shown that two different mechanisms should be distinguished by which multiple technologies can arise, i.e., from “technology-specific” or from “shared” factors, which implies a mechanism-specific set of prices, quantities and rents. We discuss and extend these characterizations, notably in relation to the real-world characterization of water as a factor (for which we use the terms technology specific, fully shared and “mixed”). We propose that the presence of these separate mechanisms results in the models being sensitive to relatively small variations in specific numerical values. To address this sensitivity, we suggest a specific role for specific (sub)models or key choices to counter unrealistic model outcomes. To support our proposal we present a selection of simulations for aggregated world regions, and show how key results concerning quantities, prices and rents can be subject to considerable change depending on the precise definitions of resource endowments and the technology-specificity of the factors. For instance, depending on the adopted water heterogeneity level, outcomes can vary from relatively low-cost solutions to higher cost ones and can even reach infeasibility. In the main model discussed here (WTM) factor prices are exogenous, which also contributes to the overall numerical sensitivity of the model. All this affects to a large extent our interpretation of the water challenges, which preferably need to be assessed in integrated frameworks, to account for the main socioeconomic variables, technologies and resources.

Keywords: resource constraints; water; world trade model; multiple technologies; scarcity rents



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1. Introduction

Global demand for water resources is steadily increasing and the water pollution problems continue to get worse [1]. The World Economic Forum signaled a water crisis and listed it as the fourth highest risk by impact [2]. The Sustainable Development Goal (SDG) 6 on clean water and sanitation [3] provides a unique opportunity to accelerate progress on Agenda 2030. As summarized in [3], water is crucial to the advancement of human rights by reducing poverty and inequality and enabling peace, justice and sustainability. Accordingly, water modeling and water research have become basic tools for analysis and understanding.

Interest in water modeling now ranges from studies of hydrological and surface water quality models [4,5], to groundwater [6], and water resources assessment models [7]. Additionally, water modeling, distancing itself from regional and basin perspectives,

now includes studies on water footprints and virtual water (VW). The concept of virtual water was coined in the early '90s by Tony Allan, analogous to the idea of embedded or embodied water, conceptualized and estimated in previous decades in environmental input–output analysis), meaning the water needed to produce a good or service through the production chain), which incorporate trade [8–10]. Accordingly, there are publications in this line, which provide policy recommendations such as producing less water intensive commodities in the severely water stressed regions. The basis for these recommendations is the indirect connection of water locally and globally [11], especially between use and scarcity through trade.

These types of studies, however, have also been subject to criticism highlighting that in the “real world” decisions are not generally based on the scarcity of resources, but are based on many economic factors and variables, and that, consequently, several factors (and not just water) play a role in determining a region’s comparative advantage [12–16] (see Section 2 on the concept). As partly reviewed by [17], these discussions have continued discussing claims on VW trade using the Heckscher–Ohlin trade model [18–21], while [22] reacted to [18] by arguing that the VW concept is consistent with comparative advantage (classical theory, which started to be developed with Ricardo 1817 [1973] [23]) as a country’s relative abundance (or scarcity) of water endowments does represent a source of comparative advantage c.q. disadvantage.

A model dealing with comparative advantage, which is particularly suited to deal with direct and indirect impacts and pressures through trade and which accounts for resource use and scarcity and/or abundance is the World Trade Model (WTM). This is an inter-regional input–output model, which captures the interactions of consumption and production in the distinguished regions. The model determines prices, regional production and inter-regional trade under constraints on production factors such as labor, capital and water [24], by minimizing the global factor costs (with exogenously given factor prices). This means that the relative scarcity of the resource under study (e.g., water) plays a role (mainly by introducing resource constraints), so that when (c.q. if) a country or region exhausts a certain resource (such as water), production needs to take place elsewhere. Similarly, in the model consideration is given to the question where it is “less costly” to produce commodities with a certain technology. According to [24], the model is able to represent “trade based on direct cost comparisons (i.e., a direct calculation of comparative advantage in the general m regions, n goods and k factors of production case), the determination of scarcity rents on fully-utilized factors, and tracking of physical quantities in physical units as well as monetary ones”.

However, the ways in which these aspects are related to the basic Ricardian notions such as comparative advantage have rarely been discussed. For example, ref. [25] reflected on the different results that may occur if one views factors as being technology specific or as shared among different technologies. A resource that is “technology specific” uses only one specific technology. If it is “shared”, it is used by more than one technology. Considering this difference, we may wonder about the role of this point when working with water resources, and the way it relates to other conceptualizations and decisions on the representation of factor use, endowments or prices.

There is another aspect. We point out that the presence of these separate mechanisms results in models being overly sensitive to relatively small variations in specific numerical values, which include data on input purity, production totals and stock data. These notions have significant effects when dealing with factors that are used in a number of different forms (such as in terms of different qualities), and that are used in different ways by economic sectors (e.g., some sectors can only use clean water). In the WTM, when dealing with water (as also in the case of certain other factors), several conceptual questions should be addressed, which, nonetheless, have only rarely been discussed. In this contribution we signal three such questions when dealing with water. These questions concern, respectively, (1) whether the (water) resources considered are technology specific or not, (2) the role of factor (i.e., water) homogeneity and (3) the question of what precisely is reflected by

exogenous (water) prices. In this article we will only briefly pay attention to the 1st and 3rd points, thereby mostly focusing on the 2nd, the homogeneity question. The idea of heterogeneity in “grades” of ore resources has been studied in [26]. Homogeneity in this context refers to the extent in which a factor (here water) can be considered to possess a uniform quality. This uniformity (or its absence) represents a realistic constraint, which, in fact, often may require further subcategorization to be properly highlighted. The underlying concern here is that, as we shall show, small changes in a factor’s composition (i.e., changes that result in certain factors factually consisting of more than one quality type) can radically change the overall picture. We show that very different results on production specialization, trade, resource use and costs are obtained with different conceptualizations and classifications of water quality types, even when data are similar or the same. The discussion of this question is extended both theoretically and empirically, illustrating what tends to occur in “minimal” and in “real world” examples. A “strategy” to address the signaled sensitivity basically suggests itself. We propose a specific role for the selection of specific (sub)models to counter unrealistic model outcomes. These (sub)models should be organized and “synchronized” with the basic model in such a way that the overall structure is more robust regarding the effects of relatively small changes than the model we started with.

The article is organized as follows. Section 2 briefly reviews the literature on comparative advantage and input–output types of studies, with a focus on the WTM and those publications that deal with water and the way in which factors can be represented. Section 3 summarizes the methodology. Section 4 conceptualizes the introduction of factors and presents the main concepts and discussions that we provide or advance on. Section 5 defines the scenarios and/or simulations, while Section 6 illustrates the results of the questions conceptually discussed with simulation examples, which highlight the very different results “*ceteris paribus*” of changes in the framing of water heterogeneity and the technology-factor relation. Section 7 extends the discussion on related issues in practical implementation, while Section 8 summarizes and presents the main conclusions, implications and possible extensions.

2. Selected Issues in the Literature on WTM, Water and Dealing with Factors

The literature on Ricardian comparative advantage (Ricardo, [1817] 1973) is vast. However, only certain aspects of this body of literature are relevant here. Among the many aspects that we cannot go into we may refer to the discussions of the extension beyond the familiar $2 \times 2 \times 2$ framework (see [27–29]).

As reviewed, e.g., in [30] and summarized in [31], basically Ricardian models are driven by differences in productivity across countries and resource constraints. Comparative advantage finds its origin in technology differences and in geography. Heckscher–Ohlin models, on the other hand, are driven by differences in factor intensity across countries. Exogenous supply differences—often skill supplies—then determine comparative advantage among countries. Regarding this, we should recall that, additionally, there also are key empirical regularities in trade that cannot be fully understood within the canonical Heckscher–Ohlin model. We refer here to the relation between trade and distance, country size, price differences, the fact that factor equalization does not seem to be confirmed empirically, and, most relevant, that productivities within the same industry appear to differ across countries. Needed here certainly is additional theory on themes like “increasing returns” or a full realization that trade specialization is at least partly based on technology differences, not simply on factor endowments.

In this context, many recent works, which model or discuss comparative advantage have introduced Ricardian aspects. However, at the same time further developments regarding factor abundance, specialization, product differentiation or specific conditions (e.g., the introduction of further complexities involving institutions, geography, etc., especially within the—new—new trade theory, see e.g., [28,32–40]), can be observed.

Within the context of input–output modeling, which allows for a detailed reflection on the interactions among different sectors and/or countries directly and indirectly, com-

comparative advantage has been studied since Leontief's famous test of the Heckscher–Ohlin theory for two countries and two factors [41]. Particularly since the 1990s, comparative advantage has been analyzed through linear programming. In [42,43] a programming framework was developed for an endogenous determination of trade based on comparative advantage by integrating an interindustry representation with standard trade assumptions. All prices are endogenous in these models, including the factor prices. This included the 2001-publication repeating Leontief's test of the Heckscher–Ohlin framework for two countries and two factors, with and without similar preferences and technologies, but (unlike Leontief) with trade flows determined endogenously on the basis of relative comparative advantage and maximization of levels of final demand. Shestalova (2001) [44] introduced an additional region, made relative world prices (but not price levels) endogenous, and used this framework to refine the measurement of total factor productivity. Interestingly, despite the enduring popularity of the concept of comparative advantage, the number of models and studies making use of the input–output frameworks in that line initiated by Leontief is not very large.

In this context, the WTM [24] took the form of a Linear Programming (LP) model of trade in a world with m regions, n goods and k factors of production. The model was put forward as based on comparative advantage as the leading principle in determining the global division of labor and prices. In this context, the model was extended with trade economics concepts (e.g., the role of factor endowments or the notion of non-traded services) and with equations that reflect real world constraints and, hence, add more realism to the baseline solutions. Later on, refs. [45,46] extended the framework to allow for the real world fact that often multiple technologies within the same industry coexist. This was called the rectangular choice of technology (RCOT) model—of an economy in which sectors can use multiple technologies, each producing the same homogeneous output. The model is presented in the next section. When factor supply is constrained, that is, if final demand cannot be sustained with the available technologies, an additional technology will enter that produces the same commodity, next to the already active technology in that sector, with the new combination minimizing overall factor cost for the economy as a whole. Hence several of these alternative technologies may, but need not, operate simultaneously.

Steenge et al., (2018) [25] exemplified a solution for a region, in which sharing of factors among technologies is allowed. Using the specification in [47] as an example, the specification of the factor input coefficients matrix (i.e., matrix F^* in the paper) is as follows: rainfed is technology specific, while irrigated land, surface water and groundwater is shared by three technologies each (one for agriculture, one for manufacturing and the last one for services), and labor and capital (shared by the seven distinguished technologies). This means that implicitly different ways of dealing with comparative advantage and scarcity were dealt with for different combinations of factors and/or technologies. In this regard, in many studies with WTM/RCOT different configurations or conceptualizations of the different factors and/or technologies [48–55] have been used, mostly without explicitly stating these differences (i.e., which factors were shared and which ones were technology specific) and the implications of this. In [26], furthermore, it was shown how technical and economic changes can impact the overall reserve estimates.

We should observe that empirical studies tend to use a combination of mechanisms depending on the subject studied. Labor and capital are standard introduced as shared factors (with perfect mobility between technologies and sectors) while other natural resources such as land (irrigated or rainfed) and, in some cases, water types are treated in these applications as technology-specific. As we shall see, this, in itself, introduces a number of specific problems.

3. Methodology

Table 1 summarizes the model parameters and variables and shows the primal and the corresponding dual of the model.

Table 1. Model parameters and variables (m regions, n sectors, t technologies (in the original WTM $t = n$, while potentially different in the rectangular choice of technology (RCOT)) and k factors of production).

	Notation	Dimension	Definition
Exogenous Parameters	\mathbf{A}_i	$n \times t$	Inter-industry inputs per unit of output in region i
	\mathbf{F}_i	$k \times t$	Inputs of factors of production per unit of output in region i
Exogenous Variables	\mathbf{y}_i	$n \times 1$	Final demand in region i , including net exports
	$\boldsymbol{\pi}_i$	$k \times 1$	Factor prices in region i
	\mathbf{f}_i	$k \times 1$	Factor endowments in region i
	\mathbf{x}_i	$t \times 1$	Sectoral output in region i
Endogenous Variables	\mathbf{p}	$n \times 1$	Commodity prices from the WTM
	\mathbf{p}_{nt}	$n \times 1$	Commodity prices from the NTM ("No-trade model", in absence of trade in region i)
	\mathbf{r}_i	$k \times 1$	Factor scarcity rents in region i
Objective Functions	Z, W	Scalars (1×1)	At optimum $Z = W$, assuring that total factor costs equal value of total final deliveries

Following Duchin (2005) [24] the formulation of the WTM (presented as a primal model) takes the following form

$$\text{Minimize } Z = \sum_i \boldsymbol{\pi}'_i \mathbf{F}_i \mathbf{x}_i \quad (1)$$

subject to

$$\sum_i (\mathbf{I} - \mathbf{A}_i) \mathbf{x}_i \geq \sum_i \mathbf{y}_i, \forall i \quad (2)$$

$$\mathbf{F}_i \mathbf{x}_i \leq \mathbf{f}_i, \forall i \quad (3)$$

$$\mathbf{p}'_{nt,i} (\mathbf{I} - \mathbf{A}_i)' \mathbf{x}_i \leq \mathbf{p}'_{nt,i} \mathbf{y}_i \quad (4)$$

$$\mathbf{x}_i \geq 0, \forall i. \quad (5)$$

Using linear programming, Equation (1) shows the objective function as minimizing the global factor use costs in monetary terms; Equation (2) guarantees that the production is sufficient to satisfy final demand; Equation (3) guarantees that factor use does not exceed the available factor endowments; Equation (4) is the benefit-of-trade constraint to make sure trade is to be preferred by requiring that the value of exports be less than the value of imports at no trade prices (which are calculated in a separate exercise where each region has to meet its own final demand without factor constraints) and Equation (5), finally, assures that production is non-negative in each region. In the case of the original RCOT, the WTM above is written in terms of \mathbf{I}^* , \mathbf{A}^* , \mathbf{F}^* and \mathbf{x}^* (to denote variables and parameters that use a technology dimension (symbol, " t ") instead of a sector dimension (symbol, " n ") in place of \mathbf{I} , \mathbf{A} , \mathbf{F} and \mathbf{x} , thereby permitting an economy to have zero options for some sectors and two or more for others in Equation (4) is not included.

The dual model can be written explicitly in the WTM (with the corresponding starred terms and without the last term for the RCOT) as:

$$\text{Maximize } Z = \mathbf{p}_i' \sum_i \mathbf{y}_i - \sum_i \mathbf{r}_i' \mathbf{f}_i - \sum_i \alpha_i (\mathbf{p}_{nt}' \mathbf{y}_i), \forall i \quad (6)$$

subject to (also, to formulate the RCOT, without the last term before the inequality)

$$(\mathbf{I} - \mathbf{A}_i)' \mathbf{p}_i - \mathbf{F}_i' \mathbf{r}_i - \alpha_i (\mathbf{I} - \mathbf{A}_i)' \mathbf{p}_{nt,i} \leq \mathbf{F}_i' \boldsymbol{\pi}_i, \forall i \quad (7)$$

$$\mathbf{p}, \mathbf{r}_i, \alpha_i \geq 0 \quad (8)$$

where α_i , a scalar, stands for the endogenously determined benefit-to-trade shadow price in region i .

The database for the simulations in Section 5 is compiled from the GTAP database [56,57] aggregated into regions, mainly similar to continents with a split of Spain from the EU. The idea is to show how the model involving differential characteristics leading to a comparative advantage may work for some large regions, but also that it may be of interest for relatively smaller countries (in terms of extension, macroeconomics, endowments, etc.), confronted with more specific water pressures (which in this case also happen to be relevant, having arid and semi-arid areas).

Along the different scenarios we show the effect of splitting water accounts from the general GTAP factor accounts, complementing it for factors, especially for water, from [54], characterized as “real world” coefficients or data (some other splits are more “naïve” or oversimplified to illustrate how these affect the results, step by step). The elaboration of sustainable endowments of water is based on the interaction of three different concepts: renewable water, exploitable resources and environmental requirements (see [50,51]), but also on the natural rates of recharge of underground aquifers, and on a more precise use of the concept “environmental requirements” to represent the demand for surface water for the conservation of riparian ecosystems [47].

In general, the scenarios introduced in Section 5 evolve from the more aggregated cases (thereby keeping prices, i.e., the $\boldsymbol{\pi}$ vector, equal to 1), to scenarios in which physical units are used, with splits that are more realistic and useful to obtain insights in comparative advantage, with several types of water uses, prices and endowments.

4. Conceptualization of Factors, in Particular of Water and Its Homogeneity

This section provides a concise description of the experimental results, their interpretation and the conclusions that can be drawn.

4.1. From Previous Literature to the Conceptualization of Factors, Especially Water; Assumptions and Classifications

As concluded in Steenge et al. (2018) [25], the increasing evidence of substantial resource scarcities requires (1) that models are developed to analyze scenarios about the future that contain factor constraints, (2) that alternative production options need to be specified to substitute or complement the original sought after lowest cost option and (3) that a mechanism is in place to induce a shift towards these alternative options.

Duchin and Levine (2011) [46] have shown how to represent and study a multitude of technologies within one region producing basically the same commodity, thereby illustrating how cheapest but comparatively less efficient technologies can be replaced over time by more expensive technologies that are more efficient in the use of the scarce resources. In this context also the prices of commodities and the appearance of rents were explained. We should recall here that in many cases the original technologies may not be replaced but often will be “still around”. Furthermore, a priori insight in which technology will be the “cheapest” one is only rarely possible. In general, we do not know which technology is more expensive by just considering the input columns. The outcome depends on the global minimization processes, so often even with shared factors we may see that some are exhausted, and that certain other technologies stay active (without replacement).

Steenge et al. (2018) [25] contextualized this and highlighted the mechanism of the coexistence of technologies, which is closer to the logic of several classical economists and of discussions (around the 1970s, by Samuelson and others) such as the non-substitution theorem. If factors are not shared, they are classified as technology specific. In that case, if scarcity sets in, we see that cheapest but efficient technologies stay around but are accompanied by more expensive and less efficient technologies. This property of the model especially becomes visible for increasing final demand (i.e., without technological changes).

As already referred to in passing in the introduction, the question of whether (water) resources are technology specific or not, is directly related to the question regarding the role of factor (water) homogeneity, which may also be extended to geographical questions. Before going into the role of water homogeneity and/or heterogeneity, we shall discuss below the entry of new technologies when constraints become binding and scarcity rents appear.

4.2. Towards Representing Water Heterogeneity and Its Endowments

As we will see in the numerical examples, water, as most other natural resources (with a few exceptions regarding land), is only rarely specifically accounted for in monetary terms as a factor of production in national accounting. In many theoretical and empirical models, as we have referred to, natural resources play a crucial role as factors of production so the first basic need is to specifically represent them individually (as land, water, oil, minerals, etc.). To what extent scarcity, production specialization and trade according to comparative advantage are reflected then, depends on properly distinguishing them. This, clearly, improves the structure of (modeled) production, i.e., the combination of an inputs' and factors' "recipe". Moving the framework from representing water with one single account to one showing several ones is evidently also linked to the number of technologies shown and on "competing" or "coexisting".

To what extent a factor, and particularly water, is considered homogeneous or not may to a very large extent determine the realism of solutions, the extent to which the scarcity factor rents appear or not, and even the feasibility of solutions. This is what we shall illustrate with a number of simulation examples in the following section, in some cases considering three qualities of water ("pure", "almost pure" and "less pure"). This classification, clearly, should be done very carefully, and be based on real world cases, since otherwise we cannot properly interpret prices, quantities and rents.

Following [58] and others one cannot always have in mind a fixed reserve base, particularly when this base changes based on the price of the resource. Springer (2011) [59] already noted that a common approach to circumvent the need to define potential quantities of regional land and water endowments is to use as the limiting constraint on production the price of economic reserves, the extraction technology available or the state of the remaining resources elsewhere. As posed by [26], one can use for the endowments constraints concepts such as forms of effective supply (e.g., the maximum capacity or technically accessible yearly flow of resource extraction). This work illustrated also the shift in the relative costs of extraction and processing technologies, which directly impacted world (ore) prices and hence the accessible reserves. There are other factors, namely land and water, which might be more context specific and their "reserves" less dependent on an international price (directly by the price of the resource, and indirectly through goods and services requiring them), and more dependent on the relation between technologies and costs, transport costs, etc. In the case of water, the "effective supply" also may consist of the sustainable endowments (exploitable resources and renewable water net of environmental requirements, see, e.g., [47,59]). If the resolution of the model is performed dynamically (step by step, year by year, see, e.g., [54]) renewable resources can be taken into account yearly with or without the sustainability constraints (depending on whether the sustainability of the solution or the realism of some contexts without them is prioritized). Exploitable resources, such as underground sources, can be limited (with a sustainable constraint) to replenishment rates, or, without such a constraint, by "out of the model"

recalculations of next year's endowments by subtracting the resources that have been exploited beyond replenishment rates.

Another issue that we will also tackle in the following subsections is to what extent endowments can be made technology specific based on the fact that only some of them can be accessed (due to location or other factors). Linking the issue again also to [47], in that work scenario analysis showed how based on economic drivers the reserves may vary over time. Here due to the particularities of water (e.g., it being less tradable, less exposed to the international prices, etc.) we approached a similar issue in an alternative way. When, for example, we find a water reserve of a type that is less accessible or more costly to extract than other, we may represent them independently with a factor specific technology (what is discussed in Sections 4.3 and 4.4), in which, for example, the transport cost or some other costs are higher for the second (and also the corresponding π_i).

Furthermore, it is worth noting that other aspects, in particular representing institutional backgrounds, affect the dimensions, quantity and quality of water availability. To start with, this reflects the importance of institutional decisions to have more (or less) water treatment, access, etc., which ultimately affects the de facto water availability of each type. However, this also reflects the fact that ultimately water rights (and sometimes related ones such as those for agricultural land and fishing), water management institutions, water boards, social norms, etc., select the spatial and temporal definitions. Theoretical and practical cases in which water resource governance (the system and structure for allocating and protecting water) is underpinned by law and other institutional regulation can be found in, e.g., [60–64]. Water Boards are, for example, organizations that also affect the de facto water availability, and other choices confronting management. Some of these date back a very long time and continue having managing power, such as, e.g., in the specific country of the database, Spain, with Europe's oldest continuing legal court called the Water Tribunal of the Valencian Plain, which keeps having customary norms of water usage for the irrigation communities (see e.g., [65]). In the Netherlands, Dutch Water Boards, dating back to medieval times, are also an example of the continuing evolution of modern water management and water policy, including the establishment of new institutions and governing bodies. Over the years, policy was organized to a very large extent around two factors, i.e., (1) the fact that almost half the country lies below sea level, and (2) the age-long policy of reclaiming land from low-lying areas ("impoldering"). These two codetermined policy at the national, regional and local levels, Water Boards having a dominant role especially in the last two. These have shaped a modern form of cogovernance between the Boards and other public authorities, thereby giving evolving issues such as environmental and groundwater concerns a more central position (see [66]).

4.3. Technologies That Can Use Several Qualities of Water; Returns and Water Treatment Technologies

The above emphasizes the importance of distinguishing heterogeneous factor (water) types (if any), so as to include more realistic factor constraints and results. Even if we would possess an ideal subdivision (say three, five or ten water quality types), Leontief types of technologies stress a fixed "recipe" of inputs needed for production. Some products might be obtained with a technology, which can use "indistinctly" several types of water quality. For example, a sector that can operate with the worst quality of water can often (without having to enter into price issues) operate with cleaner water. In the real world, if the price of the cleaner water is higher, typically the first type that is chosen will be the cheaper one (typically the lowest quality one). In this light, we would suggest that in order to incorporate this type of choice in the WTM/RCOT model, we should deal with each of these options as an "artificially" different technology in which, even if all other inputs cost the same, the same input column is employed, except for the factor input in question (the water quality type), which is technology specific. This will allow adopting one or more technologies, depending on the factor prices (again, in the context of global cost minimization). Hence, one of our recommendations will be that we should represent as many columns as "equally possible" water quality inputs.

The second aspect of the title of the subsection refers to water returns and water treatment technologies. Both aspects occur in the real world and provide more realism to the solutions, as we will see with the differential results of scenarios f1 and f2 in Section 5. Water returns (represented as negative coefficients in the **F** matrix) allow increasing the de facto water endowment of lower quality forms than the initial use. In this way columns of water treatment technologies can “capture” lower quality forms and deliver them to higher ones.

4.4. *The Role of Geography and/or Transport of Factors within Regions*

The different logics of technology-specific factors and shared factors have been clarified in [25]. Regarding the first category, we may think of a typical Ricardo situation, say a whisky industry that gets water from a nearby creek with pure water, the factor input being given by a specific coefficient. With an increase in demand, we may find that the supply of this water is running out and that additional pure water is obtained from a faraway creek and that this water costs the same at that faraway spot. Now before this water can be used it has to be transported. Assuming that transport cost is higher with distance, we may wonder how this can be represented and dealt with, particularly within the WTM/RCOT types of models. Clearly, in this case, the cost is basically connected to the factor. If the production with the different origin (creek) of pure water was represented as a different good (whisky1/whisky2) one could probably use the representation of the WTM with Bilateral Trade (BT; see [67] for the WTMBT for an interesting solution to represent the cost of transporting final goods (making use of the “Distance Matrix—*D*” and “Weight Matrix—*W*” of goods). Without the need to represent them as different goods, we believe that it is still useful to represent them with the RCOT as two different technologies, each having access only to the endowment of one creek. Regarding this, additional study of the case should decide if the situation should be represented as (1) an additional cost of transport in the appropriate input coefficient matrix (typically at the intersection of the “row of transport” with the “column of whisky”, even if it does not show specifically that it is due to water, since ultimately, it is a cost of transport, and not a further factor use) or as (2) with the same input coefficients column as under (1), but with an increasing factor cost, say with a multiplication of the factor coefficient by $t > 1$, the scalar representing the higher cost for the factor. This would support Ricardian views of comparative advantage as being linked to a distance parameter. Ideally, these cases of different distance or accessibility of factors, also should be represented as different technologies. Obviously, the degree of detail in the representation of factors and technologies needs to be weighted and/or assessed in relation to the importance for the model (its accuracy, etc.) and the possible overcomplexity and running time that it may introduce (such as in terms of its parsimony).

4.5. *The Issue of Exogenous Prices and Their Valuation*

Another important issue is the role of factor price exogeneity in a model like WTM/RCOT. Having the Leontief interpretation in mind, certain changes occur in the real or physical world (such as regarding the distribution of the net product), and after that the model is used to calculate the corresponding prices. In the WTM/RCOT model something different occurs in that exogenous prices are given a dominant influence in establishing the available choices since the objective function is the minimization of global factor cost, composed by factor use coefficients, their exogenous prices, and the production bundle itself. The logic of the exogenous prices is that say, wages are “exogenously” lower in developing countries with a large labor force, like China, than in Europe or the US, and hence labor-intensive production might (depending on the whole costs structures) move there in order to minimize global factor costs. This exogeneity is, however, far from obvious in several economic contexts. The Marshallian supply and demand schemes, e.g., may generate different prices in this respect. In a Walrasian general equilibrium context it will be the confrontation of the labor supply of, say, Chinese workers, and the demand for labor, which determine the equilibrium wage. Keynes’s theory of wages and prices contained

in the chapters 19–21 of Book V of *The General Theory* (1936) [68] is also different; wages, e.g., have an indirect effect on employment through the interest rate (the “Keynes effect”, see [69]), and so on. Already in the simulation example “d” (see Section 4) we will see how these different prices (for water) start playing a major role in decisions about the location of production. The decision regarding which factor prices are introduced or represented in the models therefore is also of prime importance.

Following the insights on income distribution in [70], the WTM/RCOT could be adapted to endogenize certain prices. Without entering in that matter here, it is worth discussing how prices are typically obtained in the WTM/RCOT literature.

In the case of labor, prices are typically obtained from wages; in the case of capital, usually from some kind of remuneration (a “rate of return”) and even for land usually some kind of information on rents or returns on land is taken. These are all “prices of exchange”, which, despite being “initial or “ex-ante”, are actually traded in “markets”. A somewhat different story is often found in the literature on the “extraction type” of resources, for which normally the cost of exploitation is taken, if available, (and otherwise some approximation of the price of the resource). For water, if there is a direct extraction, there might nevertheless not be a clear reflection of the cost of extraction (in some cases no price is paid for extracting it, so that there is no computed “factor cost” for extracting even when there should be one). Prices for water in many contexts are only paid by some of the users (technologies in the context of WTM/RCOT) and in many cases are based on regulations, which make it only partly dependent on the quality at hand (but also social concerns are involved, water being considered an essential good). The logic then is to approximate as much as possible the extraction costs even if the existing exchanges do not reflect them well.

Additionally, again, following the idea that in *f* one can define endowments, which are more or less based on sustainability (depending on what type of solution is searched), factor prices probably show similar challenges and logic regarding what is accounted for. In that sense the logic could be that if volumes for ecosystem services are subtracted from the endowment, also the pricing of factors might not have to include these non-market values.

In the case of water then the existence of “real world” exogenous factor prices is far from obvious conceptually and empirically, and as we will see in the empirical examples, will have important effects on prices (say, e.g., taking or not average world prices). As found in studies that try to attribute values to the world’s ecosystem services and natural capital (see e.g., Costanza et al., [71,72]), these types of benefits of nature for humans are huge, also if converted into monetary units and even if estimated under a number of simplifications. Even if only accounting for some kind of “market prices” of resources, e.g., of water, we would obtain relevant absolute figures in monetary units of the value of water use (and even much higher ones of endowments), which are very rarely reflected in national accounting (value added usually is only attributed to labor and capital). Typically, different prices of water do exist, which, although in some way related to quality, are rather based on the type of use (agricultural/industrial/domestic) and often based on regulations and social concerns.

Regarding the exogeneity of factor prices, a completely different approach also is worthwhile to discuss. Since the 1990s waste input–output (WIO) analysis has been steadily developed as an answer to the growing problems of the recovery and recirculation of waste materials. The WIO approach is based on a distinction of product life cycles in three tiers, i.e., production, use and end of life. This subdivision responds to the fact that each stage has its own internal structure and logic. However, recently a solid base in input–output (IO) has been established with a simultaneous interconnection with material flow analysis (MFA), see e.g., [73]; for foundations in IO analysis, see [74].

IO offers here not only the standard subdivisions into sectors, commodities, factors and the final consumption categories, but also the possibility to get insight into the structure of prices and rents and, most relevant, the option to extend the theoretical framework into

optimization and other extensions. In terms of WIO this means an extension of sector types into a number of waste categories and treatment sectors. In addition, in terms of WTM/RCOT types of modeling this means that specific policies can be considered that open up interconnections with subcategories of industrial ecology and, in a wider context, with central notions of a “circular economy”. This step also makes it possible to distinguish various “quality levels”, which, given an appropriate categorization, can provide the foundation for the introduction of “exogenous” factor prices in the WTM/RCOT family of models. In this context, the “price” of a factor would consist of the costs associated with keeping the “quality” of the factor in question at a specific level in relation to designated geographical areas and periods of time.

4.6. The Simulation Examples: Equal Representations, Feasibilities and Infeasibilities

In this final conceptual subsection, we would like to signal the existence of other relevant conceptual aspects, also illustrated by the simulation results. In several of them, we illustrate the equivalence of certain changes, e.g., splits of factors with the same factor prices, no additional scarcity being introduced, etc. However, also how, as alluded to in Section 4.2, with the representation of water heterogeneity, the world we look at and model may seem a quite different one. Indeed, in the extreme, we may move from representing seemingly unconstrained scenarios (with all available water quantities) to very constrained scenarios when taking into account the different water quality types and factor prices.

5. Scenarios and Simulations

Definition

(a) The baseline of scenario a) then follows the case presented in the Supplementary Material (Tables S1–S3), in which we had $m = 6$ regions, $n = t = 3$ goods and technologies (aggregated to Tech 1 = Agriculture; Tech 2 = Industry; Tech 3 = Services) and $k = 3$ factors of production.

(b) This scenario split from Factor 2 (which was assumed to include water resources) the Factor Water (as only one factor or type). The split assures that the sum of the coefficients of Factors 2 and 4 is equal to the former Factor 2. This was obtained by previously multiplying the water uses in physical units by the prices and aggregating, to obtain the elements of water use (in million \$), which is what was subtracted from Factor 2 in this “b” scenario (in the scenario factor prices were still assumed to be equal to 1). The large F matrix in which each of the six regions matrices F_i is represented one below the other, taking the following form in Table 2:

Table 2. F matrix of the water split of former Factor 2 into a new Factor 2 and Factor 4.

	Tech_1	Tech_2	Tech_3
Agricultural land	0.131633	0	0
Labor and Capital	0.375444	0.297183	0.592362
Other resources	0	0.009668	0
Water	0.094734	6.47×10^{-6}	1.68×10^{-5}
Agricultural land	0.083391	0	0
Labor and Capital	0.304105	0.392219	0.641501
Other resources	0	0.009477	0
Water	0.028825	0.000485	8.12×10^{-5}

Table 2. Cont.

	Tech_1	Tech_2	Tech_3
Agricultural land	0.08673	0	0
Labor and Capital	0.391501	0.391099	0.565451
Other resources	0	0.004219	0
Water	0.005841	0.000851	0.00026
Agricultural land	0.07518	0	0
Labor and Capital	0.438036	0.366987	0.633884
Other resources	0	0.002077	0
Water	0.038651	0.00063	0
Agricultural land	0.188696	0	0
Labor and Capital	0.402298	0.331826	0.604751
Other resources	0	0.033548	0
Water	0.02122	0.000194	0.001069
Agricultural land	0.11229	0	0
Labor and Capital	0.370475	0.398802	0.622043
Other resources	0	0.060001	0
Water	0.150609	0.016394	0.01895

(c) In this scenario the prices were not equal to 1, but used the “average real world” price per unit of water, obtained as a weighted average of the six regions prices (also average for a specific quality). This means that now the F matrices and f vectors were purely physical. The case was consistent in terms of endowments value with the ones above.

(d) In a fourth case, the consistency with what has been shown was preserved, but this time there were realistic prices (million $\$/\text{hm}^3 = \$/\text{m}^3$) and also realistic and (considered to be) accessible (with current technologies) physical endowments (hm^3). For the six regions the vectors took the form:

$$f_w' = [2,564,338 \quad 6,664,000 \quad 498,500 \quad 111,500 \quad 1,381,000 \quad 1,355,402] \quad (9)$$

$$\pi_w' = [0.117121 \quad 0.155179 \quad 0.220233 \quad 0.220233 \quad 0.007426 \quad 0.029182] \quad (10)$$

(e1) In this case we went back to factor prices equal to 1, but the split was performed into three different water types, hence with different endowments, which took the following form (in km^3) in Table 3:

Table 3. f_w^Q water (W) endowment and prices of the water split of Factor 4 into 3 qualities (Q), low (L), medium (M) and high (H).

	Reg_1_Asia &Oceania	Reg_2_America	Reg_3_EU	Reg_4_Spain	Reg_5_Africa	Reg_6_Rest of the World	Total
f_w^H	101	358	68	15	1	75	619
f_w^M	963	2432	52	12	120	306	3884
f_w^L	1501	3874	378	85	1260	974	8071
π_w^H	0.052	0.052	0.052	0.052	0.052	0.052	
π_w^M	0.026	0.026	0.026	0.026	0.026	0.026	
π_w^L	0.002	0.002	0.002	0.002	0.002	0.002	

The above clearly illustrates the first issue of the “homogeneity question”. Even attributing proportional uses to the endowments and the same factor prices, the fact that one divided the endowment into three parts necessarily implies a decision on whether each of these factors is shared or not among technologies. For simplicity here the split of factor

uses (the F matrices) into the three accounts was simply performed proportionally for each cell according to the share of resource endowments. In other words, this implies that each technology needs the three types of quality water, and in proportion to the endowments' availability. That is, one is already determining for each technology the proportion of each water type that is needed. In order to correct for this, we will present examples in which the technologies specifically use a factor of a particular quality type.

(e2) The split was performed again into three different water types as in “d”, but this time different prices among regions (more in line with “real world” prices) were accounted for as shown in Table 4.

Table 4. Water prices of the 3 qualities (Q) by region.

	Reg_1_Asia &Oceania	Reg_2_America	Reg_3_EU	Reg_4_Spain	Reg_5_Africa	Reg_6_Rest of the World
π_w^H	0.029	0.059	0.097	0.097	0.027	0.018
π_w^M	0.024	0.029	0.048	0.048	0.003	0.007
π_w^L	0.002	0.003	0.005	0.005	0.001	0.000

(f1) The split was performed with different relations of water coefficients (not all water types need to be used by each technology in a proportional way). Only factor “uses” (positive coefficients) and not “returns” (negative coefficients) are reflected. Table S4 shows the F matrices with these more realistic distributions of water uses, see the water endowments below. Despite this higher realism, due to aggregation issues characteristic of these relatively simple cases (aggregating several technologies into the three technologies), each technology is using more than one water quality type when typically, we would expect that some technologies (e.g., services) only would use the highest forms of water quality and cannot use lower ones.

(f2) An alternative would be to allow for water treatment sectors (see [49]). Still another alternative (to the above infeasibility) is to represent in the F matrices water returns (which may lead to negative coefficients, even after aggregating uses and returns of several technologies into these three technologies), as Table S5 shows. Hence the split in this option is performed with different relations of water coefficients (not all water types need to be used by each technology in a proportional way) making use of both alternatives to introduce flexibility. This time not only factor “uses” (positive coefficients) but also “returns” of water to lower quality forms (negative coefficients) are reflected. One would expect that “Factor_Water_H” would not have any negatives if we would only consider this feature. However, they might appear since “Tech_3” is an aggregation of sectors (services) including the water distribution and treatment sector, which, exceptionally, is the only one taking water from lower quality forms and delivering it to higher quality forms. Since returns of water are allowed to be reused, the pressure on water resources is less important, thereby possibly reducing scarcity rents and benefit of trade rents. An advantage of this representation is that it allows for having “de facto” larger endowments with the water returns, which, if based on real-world data (e.g., on the geographical conditions for availability, reusability, etc.), might better reflect the real situation (having reuses of water in some cases). This also stresses the importance of institutional characteristics and decisions, which may affect or change, within the legal framework, water quality definitions, requirements, etc., but also may affect fiscal, environmental, industrial and other policies in terms of incentives to treat water.

(f3) This scenario tries to illustrate that without the features introduced in f2) there could be infeasibilities not just not only by the lack of medium or high-quality water, but also from a lack of low-quality water (which may be difficult to explain if the problem is not the lack of total water, there being available plenty of medium-quality). In order to show it, here most (370 km³ of the current volume) of the low-quality water endowments

are “artificially” moved as medium quality for the EU. This leads to $f_w^H = 84$; $f_w^M = 422$ and $f_w^L = 8$.

(f4) We present a very simple case, which is adding from f2 to Tech 2(-1) a second technology Tech 2-2 in which in a discrete form all medium water needs of this technology are to be used as high-quality water.

(f5) In the opposite case, f5, all medium water needs of this technology are allowed to be used as low-quality water.

(f6) Now from f2, we might represent that the case in the real world is that what we have shown as high-quality water requirements in f2 are indeed a technology specific factor. A type of water that can only be used by that Tech 2-2 (given its location/technology needed for extraction/etc.). This is represented with an additional row (even with the same exogenous price), also with an additional endowment (assumed to be 30% of the high-quality endowment in all regions). That is to say, the technology is even assumed to have the same structure, but being the only one capable of using that new high quality water factor (and not using the previous high quality water factor).

What interests us is that a change in final demand may de facto change to a large extent how we see comparative advantage and derived changes. If actually the real-world situation would be as f6, in which there is a separate and technology-specific water pool or reserve, by making this set a shared factor we would not only be altering this baseline, but quite importantly the implications of a future scenario. Let's consider an increase in final demand in Sector 2 of 10% from both f2 and f6 in the following 2 simulations.

(f7) provides the result with the technology shared factors (i.e., increasing 10% of the final demand of Sector 2 from f2).

(f8) provides the result with the technology specific factors (i.e., increasing 10% of the final demand of Sector 2 from f6).

(g) Departing from the example f2, the question presented in Section 4.4 regarding the nearby and faraway creek can be addressed here in the context of accounting for additional -more inaccessible- endowments. This relates to issues addressed in Section 4.2 and in Section 7) and could be also conceptualized to consider not only a less accessible resource due to physical variables, but also institutional ones (e.g., bureaucratic difficulties to extract it, etc.). We might consider the fact that the realistic physical endowments of previous subsections are based on water resources data (FAO, 2020), but exclude what can be “reasonably” called inaccessible water with current technologies (in the Amazon, the Zaire-Congo basin, etc., following, e.g., Jackson et al., 2001). However, one may wish to add the possibility of those existing resources, thereby adding to this endowment. In simple examples as this one it is relatively easy to consider this appropriately representing the technologies that can use it. Here we might think that it is only Tech 1 that can use it (so now we had Tech 1-1 and Tech 1-2). Introducing it properly also requires that the endowment enters as a separate set (otherwise we would be increasing the endowment, which the original Tech 1-1 can use without further cost).

(g1) Option 1 implies reflecting it as an additional cost of transport in the input coefficient matrix (typically at the element where the row of transport—within Sector 2—crosses the column of Tech 1-2, even if it does not reflect specifically that it is due to water, since ultimately, it is a cost of transport, and not a further factor use). We also add a vector of “Factor_Water_L_inaccessible (LI)” with an additional endowment of 20%, the “Factor_Water_L”. We add in F an additional row with the same coefficients for Tech 1-1 and Tech 1-2 as in “Factor_Water_L”.

(g2) Option 2 maintains the same input coefficients column but shows an increasing factor cost, with a multiplication of the factor coefficient by t , the scalar of higher cost for the factor, with $t > 1$. We leave the A matrices intact and in the F matrices the cells of “Factor_Water_LI” Tech 1-2 increase by 10% with respect to “Factor_Water_L”.

(g3) Here we discuss the role of removing the factor endowments constraints.

(g4) Here we discuss the role of removing the benefit of trade constraints (bot).

Table 5 summarizes the naming of all the above scenarios.

Table 5. Summary of scenarios.

N	Scenario
(a)	Baseline
(b1)	Water split 1 account (monetary, $\pi_w = 1$)
(b2)	Water split H M L equal (monetary, $\pi_w = 1$)
(c)	Water split 1 account (physical, $\pi_w = \text{World Average Price}$)
(d)	Water split 1 account (physical, $\pi_w = \text{differential price}$)
(e1)	Water split H M L equal coefs. (physical, $\pi_w = \text{World Average Price}$)
(e2)	Water split H M L equal coefs. (physical, $\pi_w = \text{differential price}$)
(f1)	Water split H M L real world coefs. (physical, $\pi_w = \text{differential price}$)
(f2)	Water split H M L real world coefs and Water Returns (physical, $\pi_w = \text{diff.}$)
(f2*)	Water split H M L1, L2, L3 real world coefs and Water Returns (physical, $\pi_w = \text{diff.}$)
(f3)	Water split H M L real world coefs. (physical, $\pi_w = \text{differential price}$). Most low-quality water endowment as medium quality for EU
(f4)	Water split H M L real world coefs. with 2 technologies to produce 2, medium water needs as high (physical, $\pi_w = \text{differential price}$)
(f5)	Water split H M L real world coefs. with 2 technologies to produce 2, medium water needs as low (physical, $\pi_w = \text{differential price}$)
(f6)	Water split H M L real world coefs. with 2 technologies to produce 2, technology-specific factor (physical, $\pi_w = \text{differential price}$)
(f7)	Water split H M L real world coefs. 2 tech. to produce 2, technology-shared factor, $\uparrow 10\% y_2$ (physical, $\pi_w = \text{differential price}$)
(f8)	Water split H M L real world coefs. 2 tech. to produce 2, technology-specific factor, $\uparrow 10\% y_2$ (physical, $\pi_w = \text{differential price}$)
(g1)	f2 + LI; transport use $\uparrow 5\%$ with respect to that of Tech 1-1 for Tech 1-2
(g2)	f2 + LI; Factor_Water_LI $\uparrow 10\%$ with respect to Factor_Water_L for Tech 1-2
(g3)	f2 + NoFactorConstraints; Water split H M L real world coefs and Water Returns (physical, $\pi_w = \text{diff.}$)
(g4)	f2 + NoBotConstraints; Water split H M L real world coefs and Water Returns (physical, $\pi_w = \text{diff.}$)

* Note: H, M and L stand for High, Medium, Low quality water; Tech. for technology; coefs. for coefficients.

In the following section we expanded on the conceptualization of factors (in relation to homogeneity, factor prices, endowments, etc.), with different aspects to consider, some of which particularly apply to water, and which will be illustrated through the simulation results.

6. Results

(a) The solution obtained with the initial case presented in the Supplementary Material shows that, in any case, some goods are traded. Notwithstanding, there are no clear-cut skewed productions (i.e., the total production of a good does not occur in only one place) and scarcity rents are relatively low (as we will see in the Summary Table at the end of the section). The output baseline solution is shown in Table 6.

Table 6. Baseline. Solution of x (output) by region and technology (million \$).

	Tech_1	Tech_2	Tech_3
Region_1_Asia&Oceania	2,152,421	24,333,408	27,688,467
Region_2_America	1,157,388	24,882,617	29,378,990
Region_3_EU	1,177,535	19,762,573	18,495,647
Region_4_Spain	86,596	1,620,930	1,302,922
Region_5_Africa	1,040,396	6,355,317	3,093,182
Region_6_Rest of the World	0	0	3,291,771
Total	5,614,336	76,954,844	83,250,978

Source: Simulation results.

(b) We see that given the aggregation of technologies here, labor and capital are shown as fully shared factors (and in general also the aggregate of “water”), while agricultural land is technology specific (associated with the “agriculture technology”). As said before, we cannot go very deeply into the details of these categorizations, but in general “fully shared” factors tend to be factors that can relatively easily move across technologies. If we had used the fully-fledged IO data without aggregation, in which more technologies are used, we could have seen how labor_capital is still a fully shared factor, while in fact most other are “mixed” factors, being shared among only a selected set of technologies (e.g., agricultural land being shared among several technologies in agriculture).

Factor prices (as represented by the π vector) are still equal to 1 (including that of water) in our example here. In this case, the solution is exactly the same as sub “a”, since this split does not create additional constraints (although theoretically it could). In a similar case (we may call it b2), there is a distinction between three water qualities, with prices equal to 1, while factor uses are assumed to be proportional to the proportions of endowments of these three qualities. In other words, the break does not introduce any new particular further constraint for any of the three qualities. The case is consistent with (all of) the above and accordingly the solution is identical.

(c) The solution in this case interestingly already implies some small reductions in global factor cost. The main reason is that the equivalence of cases is performed having the same value of endowments (i.e., the physical endowment f_w times the prices of the factor π_w).

(d) As we show in Table 7 below, this example (as in “c”), creates changes in the distribution of production. Region_1_Asia&Oceania notably decreases its production in “Tech 1—of good 1” and “Tech 2—of good 2”, while increasing “Tech 3—good 3” (however the balance shows a decrease in production). The production of good 1 that is reduced in “Region_1_Asia&Oceania” is basically increased in “R6_Rest of the World”, which was not producing Tech 1 or Tech 2 in the previous example. The “average price” of water is smaller in this region, and Tech 1 (agriculture) is clearly the one requiring it more. With this change, other productions are also altered, e.g., Tech 2 moves out of region “4_Spain” while more of Tech 3 is produced there (the balance being provided by a decrease in production).

In order to minimize global factor costs, different water prices are used. It turns out that global factor cost decreases when we possess the (more in accordance with the real world) water prices across regions. With the reorganization of production (due to different “exogenous prices” and virtual water trade) increases, the Region_6_RestofWorld reduces much of its trade, being more self-sufficient. In this “d” case factors 1 and 3 continue being fully utilized while in certain regions scarcity rents appear, but they are slightly lower than in examples a) to c); see the details in the summary table at the end of the section). The output solution is shown in Table 7.

Table 7. Water split 1 account. Solution of x by region and technology (million \$).

	Tech_1	Tech_2	Tech_3
Region_1_Asia&Oceania	1,776,709	22,800,303	28,864,326
Region_2_America	1,157,388	24,882,617	29,377,180
Region_3_EU	1,177,535	19,762,573	18,489,859
Region_4_Spain	86,596	0	2,248,428
Region_5_Africa	1,040,396	6,355,317	3,093,107
Region_6_Rest of the World	343,011	2,585,992	1,066,403
Total	5,581,635	76,386,801	83,139,302

Source: Simulation results.

(e1) The results of this scenario could reveal changes similar to those described up to “c”, but it can also (already) create a different result as shown in the example, with higher scarcity rents due to exhausting one of the types of water quality. Indeed, as we find, the solution can even be infeasible.

(e2) The “loss” of flexibility (example “e”) is theoretically countered with the possible “gains” from taking gain of different prices across regions. Still, as we see below, the “run” is infeasible as well.

(f1) With the F matrices as specified, the outcome appears to be infeasible. When exploring solutions close to the infeasibility area, we observe that very high rents appear for the EU for the medium quality water type (which is mainly used by “Tech_2—Industries”) and to a lower extent the high-quality water type (which is mainly used by “Tech_3—Services”). This may hint towards key water constraints there without the features introduced in f2.

(f2) The result incorporates slightly higher rents, but much smaller “benefit of trade” rents. Ultimately, the representation of water treatment sectors and uses with returns in the model seems to favor (and provide) more realistic results especially in the EU, with intensive use of these processes.

Compared to the results of Table 6 (in which there was a world average price and hence no possible taking advantage of different prices among regions), in Table 8 we may see that the EU produces here much less with Tech_2 (15,685,290 vs. formerly 19,762,573). Clearly this technology requires important volumes of water, with a relatively high price in the EU), while this production is increased by Asia&Oceania (27,740,108 vs. 22,800,303). On the other hand, the EU increases its production in Tech_3 (for which it has certain specializations, high endowments of the high-water quality, etc.). In addition, we might see some increase in the production of Tech_1 in Asia&Oceania (1,887,739 vs. 1,776,709, which also reduced production of Tech_3), while some decreases were found in the Rest of the World in this Tech_1 (which slightly increased production of Tech_3).

Table 8. Water split High, Medium, Low real world coefficients and water returns. Solution of x by region and technology (million \$).

	Tech_1	Tech_2	Tech_3
Region_1_Asia&Oceania	1,887,739	27,740,108	26,192,659
Region_2_America	1,157,388	24,882,617	29,377,180
Region_3_EU	1,177,535	15,685,290	21,349,438
Region_4_Spain	86,596	0	2,248,428
Region_5_Africa	1,040,396	6,355,317	3,093,107
Region_6_Rest of the World	315,507	2,585,992	1,096,393
Total	5,665,161	77,249,323	83,357,204

Source: Simulation results.

We should stress here again that the question of the conceptualization of water heterogeneity in relation to the role of technology-specific factors plays a crucial role. Simply the fact that low quality water is split into 3 types (L1, L2, L3), each of which can be used by each of the three sectors, with endowments proportional to the f2 solution, led to higher factor scarcity rents and global factors costs (f2*, not shown for length issues) (Table 9). This already points towards the fact that these results might be much more different if further heterogeneity based on real world data would be introduced (e.g., 5–6 water classes based on water quality parameters in line with [75,76], or even in line with [77,78] with dozens of classes or classifications, thereby also distinguishing groundwater and surface quality types, which also imply different spatial–temporal endowments).

Table 9. Water split H M L, 2 technologies, M as H. Solution of x by region and technology (million \$).

	Tech_1	Tech_2-1	Tech_2-2	Tech_3
Region_1_Asia&Oceania	1,887,739	27,740,108	0	26,192,659
Region_2_America	1,157,388	24,882,617	0	29,377,180
Region_3_EU	1,177,535	15,685,290	0	21,349,438
Region_4_Spain	86,596	0	0	2,248,428
Region_5_Africa	1,040,396	6,355,317	0	3,093,107
Region_6_Rest of the World	315,507	2,585,992	0	1,096,393
Total	5,665,161	77,249,323	0	83,357,204

Source: Simulation results.

(f3) As in f1, this scenario originates from a lack of low-quality water, something that is difficult to explain in the real world if the problem is not due to a lack of total water, but due to a lack of low-quality water, there being available plenty of medium-quality. This emphasizes the importance of the features introduced in f2.

(f4) We presented a very simple case, which is adding to Tech 2(-1) a second technology Tech 2-2 in which in a discrete form all medium water needs of this technology need to be used as high-quality water. The flexibility introduced by the new technology could allow a lower cost solution, but in this case this technology is not chosen, and the solution is equal to f2.

An alternative and more comprehensive approach to represent water returns and reuses could be the characterization of byproducts and waste, which allows the simultaneous production of multiple outputs [79]. Waste activities do not have coefficients in the row (since waste per unit output is endogenous), there is no overproduction because an activity is assumed to be able to perfectly adapt the production of byproducts to the demand. Additionally, in the framework of [80] waste activities must have balanced inputs and outputs, including the treated waste flows, where we summed that the level of byproduction is proportional to the output of principal productions (there are endogenous matrices of technical coefficients and there can be an excess of production).

(f5) In the opposite case to f4, all medium water needs of this technology are allowed to be used as low-quality water. In the results, this second option reduces the global costs (Table 10).

Table 10. Water split H M L, 2 technologies, M as L. Solution of x by region and technology (million \$).

	Tech_1	Tech_2-1	Tech_2-2	Tech_3
Region_1_Asia&Oceania	1,954,571	0	27,738,774	26,124,518
Region_2_America	1,157,388	0	24,882,617	29,394,017
Region_3_EU	1,177,535	15,685,290	0	21,349,438
Region_4_Spain	86,596	0	0	2,248,155
Region_5_Africa	1,040,396	6,355,317	0	3,093,107
Region_6_Rest of the World	246,290	0	2,585,992	1,144,092
Total	5,662,776	22,040,607	55,207,383	83,353,328

Source: Simulation results.

(f6) Interestingly this change, i.e., the fact that an additional technology is factor specific and that the endowments are different, already reduces the scarcity rents and global costs (see particularly the difference with respect to f4). The different result with respect to f2 that we see is obviously somehow arbitrary, in the sense that it depends on precision in defining these variables (e.g., on the water endowment of each water factor). However, what interests us is that a change in final demand may change greatly how we see comparative advantage depending on the technology-factor specification (Table 11).

Table 11. Technology-specific factor, Solution of x by region and technology (million \$).

	Tech_1	Tech_2-1	Tech_2-2	Tech_3
Region_1_Asia&Oceania	1,803,194	22,800,361	0	28,837,389
Region_2_America	1,157,388	24,882,617	0	29,377,180
Region_3_EU	1,177,535	9,650,600	10,111,972	18,489,859
Region_4_Spain	86,596	0	0	2,248,428
Region_5_Africa	1,040,396	4,530,567	1,824,750	3,093,107
Region_6_Rest of the World	315,629	1,837,093	748,899	1,091,687
Total	5,580,738	63,701,238	12,685,621	83,137,649

Source: Simulation results.

(f7) Provides the result with the technology-shared factors (i.e., an increase of 10% of the final demand of Sector 2 from f2). The increase did not “force” Tech_2-2 to enter into production (Table 12).

Table 12. Technology-shared factor, $\uparrow 10\%$ y_2 . x by region and technology (million \$).

	Tech_1	Tech_2-1	Tech_2-2	Tech_3
Region_1_Asia&Oceania	2,153,878	35,924,706	0	23,423,201
Region_2_America	1,157,388	24,882,617	0	30,760,168
Region_3_EU	1,177,535	14,530,912	0	23,427,431
Region_4_Spain	86,596	0	0	2,342,188
Region_5_Africa	1,040,396	6,355,317	0	3,470,889
Region_6_Rest of the World	311,091	2,585,992	0	1,267,125
Total	5,926,883	84,279,544	0	84,691,003

Source: Simulation results.

(f8) Provides the result with the technology-specific factors (i.e., an increase of 10% of the final demand of Sector 2 from f6). This revealed the importance of shared vs. specific factors classification (Table 13).

Table 13. Technology-specific factor, $\uparrow 10\%$ y2. x by region and technology (million \$).

	Tech_1	Tech_2-1	Tech_2-2	Tech_3
Region_1_Asia&Oceania	2,045,395	29,586,396	0	26,816,720
Region_2_America	1,157,388	24,882,617	0	30,760,168
Region_3_EU	1,177,535	9,650,600	10,111,972	19,758,235
Region_4_Spain	86,596	0	0	2,342,188
Region_5_Africa	1,040,396	4,530,567	1,824,750	3,470,889
Region_6_Rest of the World	311,247	1,837,093	748,899	1,261,086
Total	5,818,557	70,487,273	12,685,621	84,409,286

Source: Simulation results.

(g1) The result of option 1 was a slightly smaller objective function, with smaller factor rents. Despite being “more costly” (in terms of transport input for Tech 1-2), due, e.g., to the different prices across regions, it may still be the case that it is profitable to extract and/or use the “inaccessible” water (“Factor_Water_LI”) in one region. In particular in our f2 example “Region_6_Rest of World” was already obtaining “Factor_Water_L” rents due to factor exhaustion. In this case the part of the “Factor_Water_LI” endowment is used in this region and the factor rent reduced.

(g2) The result of option 2 is a slightly smaller objective function (smaller even than g1), with smaller factor and also “benefit of trade” rents (less of a rent is needed so that sectors not benefiting from trade -but being desirable globally- enter into trade). Despite the “more costly” (in terms of use) factor of the “inaccessible” water (“Factor_Water_LI”) it is again profitable to extract and/or use it in one region.

(g3) Removing the factor endowment constraint implies that the important constraints affecting factor 1 (i.e., mainly Region_5_Africa and Region_3_EU) are removed. Something similar is valid for smaller factor rents obtained from water constraints and on constraints on other resources other than agricultural land, water and capital and labor. Specialization becomes easier and we can see how most regions end up producing one or at most two goods (with their respective technologies). It seems clear that the most water-intensive sector, Tech_1 (agriculture) without factor constraints would produce all that is needed in Region_5_Africa. Obviously before extracting conclusions for the real world, this needs to be put in the context of the great aggregations and the stylized example used here. Nonetheless, it shows clearly the logic of the way in which these type of optimization models may work. Still in some explorations that we have done with more extensive and disaggregated real world data the result seemed to point to a situation in which some developing countries are clear-cut low-cost producers, which, nevertheless, do not lead in the production of relatively primary goods due to factor constraints, e.g., on capital (Table 14).

Table 14. f2 + no factor constraints. Solution of x by region and technology (million \$).

	Tech_1	Tech_2	Tech_3
Region_1_Asia&Oceania	0	82,006,335	0
Region_2_America	0	0	45,748,414
Region_3_EU	0	0	33,368,123
Region_4_Spain	0	0	2,328,468
Region_5_Africa	6,241,443	3,043,714	0
Region_6_Rest of the World	0	950,129	2,115,264
Total	6,241,443	86,000,178	83,560,269

Source: Simulation results.

(g4) Removing the bot constraint also admitted slightly more skewed or corner solutions than f2 (with some combinations of country-technology that are 0). Factor rents slightly rose, but the optimal solution provided a lower value of Z than f2 (still it was higher than when the factor constraints were removed) (Table 15).

Table 15. f2 + no bot constraints. Solution of x by region and technology (million \$).

	Tech_1	Tech_2	Tech_3
Region_1_Asia&Oceania	1,735,684	32,840,463	28,195,071
Region_2_America	1,157,388	24,882,617	38,582,478
Region_3_EU	1,177,535	19,762,573	14,009,938
Region_4_Spain	86,596	0	2,259,173
Region_5_Africa	1,040,396	0	0
Region_6_Rest of the World	343,011	0	0
Total	5,540,609	77,485,653	83,046,659

Source: Simulation results.

Table 16 summarizes the results for each of the scenarios.

Table 16. Summary of results for each of the scenarios (million \$).

N	Scenario	Z	py	rf	bot
(a)	Baseline	81,779,281	84,561,239	351,623	2,430,335
(b1)	Water split 1 account (monetary, $\pi_w = 1$)	81,779,281	84,561,239	351,623	2,430,335
(b2)	Water split H M L equal (monetary, $\pi_w = 1$)	81,779,281	84,561,239	351,623	2,430,335
(c)	Water split 1 account (physical, $\pi_w =$ World Average Price)	81,786,541	84,561,239	342,951	2,431,746
(d)	Water split 1 account (physical, $\pi_w =$ differential price)	81,730,263	82,684,143	346,677	607,203
(e1)	Water split H M L equal coeffs. (physical, $\pi_w =$ World Average Price)	Infeasible solution			
(e2)	Water split H M L equal coeffs. (physical, $\pi_w =$ differential price)	Infeasible solution			
(f1)	Water split H M L real world coeffs. (physical, $\pi_w =$ differential price)	Infeasible solution			
(f2)	Water split H M L real world coeffs and Water Returns (physical, $\pi_w =$ diff.)	81,734,750	82,888,483	369,598	784,135
(f2*)	Water split H M L1, L2, L3 real world coeffs and Water Returns (physical, $\pi_w =$ diff.)	81,752,895	82,223,853	470,958	784,646
(f3)	Water split H M L real world coeffs. (physical, $\pi_w =$ differential price). Most low-quality water endowment as medium quality for EU	Infeasible solution			
(f4)	Water split H M L real world coeffs. with 2 technologies to produce 2, medium water needs as high (physical, $\pi_w =$ differential price)	81,734,750	82,888,483	369,598	784,135
(f5)	Water split H M L real world coeffs. with 2 technologies to produce 2, medium water needs as low (physical, $\pi_w =$ differential price)	81,648,338	82,867,597	428,815	790,444

Table 16. Cont.

N	Scenario	Z	py	rf	bot
(f6)	Water split H M L real world coefs. with 2 technologies to produce 2, technology-specific factor (physical, π_w = differential price)	81,731,863	82,888,483	350,984	805,635
(f7)	Water split H M L real world coefs. 2 tech. to produce 2, technology-shared factor, $\uparrow 10\%$ y_2 (physical, π_w = differential price)	84,763,654	85,945,818	369,598	812,566
(f8)	Water split H M L real world coefs. 2 tech. to produce 2, technology-specific factor, $\uparrow 10\%$ y_2 (physical, π_w = differential price)	84,759,950	85,945,818	350,984	834,884
(g1)	f2 + LI; transport use $\uparrow 5\%$ with respect to that of Tech 1-1 for Tech 1-2	81,733,676	82,751,923	366,689	651,558
(g2)	f2 + LI; Factor_Water_LI $\uparrow 10\%$ with respect to Factor_Water_L for Tech 1-2	81,733,171	82,687,817	365,323	589,322
(g3)	f2 + NoFactorConstraints; Water split H M L real world coefs and Water Returns (physical, π_w = diff.)	81,451,965	82,079,090	0	627,125
(g4)	f2 + NoBotConstraints; Water split H M L real world coefs and Water Returns (physical, π_w = diff.)	81,709,343	82,093,022	383,679	0

Source: Simulation results.

7. Further Issues in Practical Implementation

The examples above involve a number of aspects that are important for interpreting the outcomes (in terms of production, water uses, virtual water trade, water scarcity rents, etc.), but, for various reasons, may need additional attention for a full understanding of the model. In this section we shall take a closer look at some of these.

7.1. Transformations and Additions

First, the LP (WTM/RCOT) model provided meaningful and useful solutions in a multiregional setting using various **A** and **F** column structures that were calculated using technology and policy-based assumptions and scenarios. The consequence of this, however, is that the column totals did not add up to 1. The background here is that the standard calculation of the **A** and **F** columns (dividing each element of the matrices by totals) results in column totals of 1. This procedure, unfortunately, suppresses any notion of possible comparative advantage(s) and results in degenerate (trivial) solutions in which any combination is basically equally plausible. We should note here that, nonetheless, in some cases the above examples already incorporated additional information on factor use, even when factor prices were kept at 1, for simplicity.

The explanation of the presence of solutions (for different countries) to produce one or more specific goods or services often lies in the fact that additional transformations or additions have been put in place (a fact which WTM users tend to do). The first ones have to do with the incorporation of (natural) resources. By converting or simply substituting some of the corresponding input vectors into physical quantities, more resources are included in the **F** matrix than the ones normally captured. This de facto modifies the technology (the column input coefficients of **F**) and hence also “which country produces what”. The role of profits is most interesting, especially regarding the question how considering them (or not) in the **F** matrix can further explain comparative advantage. Although this indeed is a most interesting point, considering how resources (factors) are rewarded (labor/capital compensation, etc.), for reasons of space we focused here on how water plays an important role in reflecting the reality of factor use per unit of output (the **F** matrix) and of the endowments (the **f** vector). In particular, we saw examples of how real world reflection (via heterogeneous qualities) may even lead to infeasibilities. That is, without considering other aspects such as water treatment options [49] or further flexibility or slacks (e.g., a

further sharing of factors among regions, which is dealt with in [81]), it is not possible to satisfy the current demands with production in the different regions.

7.2. Resource Constraints

Another consideration has to do with the realism of resource constraints. As pointed out earlier, related to this is the question if one would like to proceed towards a more “real-world” solution (with tighter constraints) or rather towards a “purer”, comparative advantage one. To be sure, even after transformations of the type referred to in the above subsection, a pure LP (WTM) solution might (still) provide some sort of skewed solutions in which the “low-cost producer” region would produce most of a good or sector, thereby generating some initial (baseline) result very different from the real-world production and trade flows. Such a solution is, nonetheless, most interesting and instructive in the sense that it may reveal the “pure” comparative advantage of countries in the provision of certain goods and services, something in which many (especially trade theory) economists have been highly interested in for a long time. In that regard, it could be said that the WTM, by being able to generate and highlight these “extreme” solutions, is showing us directions in which a more efficient world economy might move. However, also this point we have to leave for later work.

Increasing the Number of Constraints

In the other extreme, one could start from a perfectly matched baseline scenario (a scenario that perfectly reproduces in the baseline year all macromagnitudes and trade flows), simply by increasing the number of constraints. These might involve some realistic biophysical constraints, labor constraints based on the active population of the country with some slack by allowing interregional migration, or incorporate capital constraints based on the existing levels of investments and gross capital formation of a country, also with some slack and the ability to move freely across sectors.

However, in order to completely match the baseline scenario, one would most likely also need to introduce additional “unrealistic” constraints. The perfectly but “artificially” matched baseline scenario would present many problems in the scenarios, the central one most likely being the inability to learn anything instructive for real world strategic planning and policymaking. In this regard, most changes obtained in the scenario would be due to the need for relaxing these constraints to get feasible solutions when changing the scenarios, and not be due to changes in the other projected variables themselves (where also the scarcity rents would have been initially “artificially” high).

In general, constraints play a role to the extent that they are based on data and considered to be realistic. In this regard, over the years a great deal of effort was put into finding the most appropriate options, e.g., of water endowments selected based on the accessible resources (under certain/current technologies and prices) to define the maximum available flows (typically sustainably) yearly. In the case of water, for example, we argue in general for working with large databases (a high number of sectors, technologies, factors, etc.) and for avoiding considering inaccessible water (e.g., by following Jackson et al. 2001, [82]). Decisions not only include the possible exclusion of physically inaccessible areas (under current technologies), but also the institutional constraints affecting them. We may think here of riparian water rights, which allocate water among the land owners along its path, water board organizations, which decide on access and/or extraction regulations, etc.). Including these in the various decision levels will definitely increase the realism of the baseline solutions. In this regard, water resource constraints also play a role in avoiding both trivial and unrealistic solutions by adding real world constraints (via the f vector), which limits the ability of a country to produce “all” world production of a good/industry (or any too skewed solution). However, we also showed how we might consider less accessible resources (which is especially useful also for other resources that require more costly technologies to get to less accessible areas, such as oil), thereby allowing for the existence of alternative, more costly technologies.

Finally, another type of constraint that one may consider is one on trade for non-traded or only partially traded sectors. In this regard, as shown by a number of studies in international economics, many services tend to be non-traded and hence a “free LP” solution would have been unrealistic. To be sure, this is a feature that can be introduced in the WTM with bilateral trade ([67], by making it expensive to “transport” those services or, in general, to transport “heavy goods” (which goes in line with “iceberg” types of transport models, see [83,84] where transport costs grow with distance, and depend on the volume of the good itself, rather than on other resources). For the case of water, “services” tend to involve consumers of small volumes of water, although typically of the highest quality. Therefore, this question might only affect the results if the modeling of the water resources is such that it distinguishes with precision this type of purified water, a situation that typically is more important for regions that have important volumes of water but of relatively low quality (one may think here of particular areas in India, Southeast Asia or Africa).

7.3. Aggregation versus Disaggregation

Finally, as follows from the employed type of regional distinction, the WTM/RCOT type of modeling is highly dependent on the levels of aggregation and/or disaggregation, particularly of sectors and of regions (see on the aggregation biases [85–94]). Typically, in input–output analysis there exist many arguments in favor of having more (rather than less) disaggregation (see e.g., [95]), if computing capabilities or other specific aspects (e.g., possible misrepresentations of the technologies due to less reliable data) do not prevent this.

On the one hand, for a full understanding, accounting for regional differences in endowments is definitely necessary. For example, if Japan is joined with other Asian countries (as in the examples presented), this results in a situation without (or with less realistic) constraints for them, e.g., on water, cropland or pastureland. On the other hand, a very specific country or even subnational data may seem ideal, but it may also lead to unacceptable results, driven by the problem of bad representation of technologies in specific countries and by trying to represent trade for which comparative advantage notions do not provide a possible explanation. The main reason for finding anomalous specializations is the fact that some technologies (columns of the input–output tables) are sometimes not well defined when a production is highly marginal or almost non-existent in a region. If, e.g., one of the main inputs is underrepresented this may lead to presenting the combination as an efficient/low-cost producer and in unrealistically assigning high levels of production there.

In this regard, for about 20 regions in the world (quite different in terms of biophysics and socioeconomics) we have found (e.g., in [54] and derived analyses) relatively robust baselines, which reproduce quite accurately real-world patterns of production, without “artificially constraining the model”. This is due to the fact that it allows for realistic factor endowments (as indicated, with several categories of water, but also employment, land types, etc.) while not falling into the issues of misrepresentation of technologies.

7.4. Additional Options

Additional options can exist in modeling trade and related issues. We may think here, e.g., of modeling the extent in which trade deficits are allowed. It will be clear, however, that this type of models cannot capture all complexities and exceptions. For example, the structural trade deficit of the US cannot be separated from the fact that the world wants to hold the dollar as a reserve currency. Evidently, unless specifically specified, this is not captured in the empirical results). This then, taken together, concerns the inefficiencies and arbitrary political decisions, which impose conditions, temporally but not consistently, or are based, otherwise, on some specific economic logic or theory. The same is true for certain other areas; this type of modeling, e.g., cannot capture properly many financial aspects. Still, all in all, virtual water resources, footprints, water scarcity, etc., can be studied with these types of modeling, thereby moving from conclusions or claims that “water scarce countries should produce less water intensive crops, and import them” to understanding virtual water patterns, the logics and drivers of change, reasons for finding scarcity, virtual

water trade according to water scarcity and so on. This implies taking into account the different options of analysis and considerations shown and discussed.

We propose that the presence of these separate mechanisms results in the models being sensitive to relatively small variations in specific numerical values. To address this sensitivity, we suggest a specific role for the selection of specific (sub)models and key choices to counter unrealistic model outcomes.

8. Summary and Conclusions

We started by signaling how water modeling and management has evolved towards understanding that local challenges are strongly connected with other places in an increasingly interconnected and globalized world. We also saw that most discussions of virtual water and water footprints have faced conceptual and empirical critiques and challenges regarding how they deal with the fact that many other socioeconomic aspects, and notably other (than water) natural resources and factors of production, play a role in the decisions on production, trade, consumption, etc. All these points towards the use of multiregional and multisectoral (commodity) models, which are able to capture those interconnections, and factor use and their scarcity. Above we tried to show that this type of models can be very useful for water and virtual water experts interested in understanding why and how specialization and trade originate.

For those trying to compare the net virtual water trade with the availability of resources—and thereby often find paradoxes—especially the results on factor uses and scarcity rents can be most important to further understand why a certain region becomes a net exporter and/or importer of certain (e.g., water-intense) goods. On the other hand, for experts on water quality, pollution, etc., some of these insights may be of considerable use. However, probably of even greater use is the knowledge that—despite the many indicators they usually work with in water pollution cases (which makes synthesizing difficult)—classifying the endowments according to quality classes (e.g., from the main parameters or water quality Indexes) is of great importance for future environmental economics modeling.

Within such frameworks, which we particularized here making use of the World Trade Model (WTM), the question to which extent a factor, and particularly water, is considered homogeneous—or not—may to a very large extent determine the realism of the solutions, the extent in which scarcity factor rents appear or not, and even the feasibility of solutions. Conceptually we discussed several situations in which we recommended representing different situations with more “technologies of production” to properly capture different costs, different options of water quality used, etc. The examples presented were also simplified to show how properly defined water resource use may modify the actual results from seemingly unconstrained solutions to highly constrained and even infeasible solutions. Similarly, the examples illustrated how different choices made in modeling or in specific policy or institutional contexts may (very) significantly affect the resource dimensions and the solutions found. In other words, we showed in which directions results on production specialization, trade, resources use and costs can be obtained employing different conceptualizations and classifications of water quality types, even when background data is similar or even the same.

A central point within the overall context of our approach was the observation that the simultaneous presence of several mechanisms to select technologies (and to interpret prices, quantities and rents) makes the models overly sensitive to shifts in the numerical values of the variables in question. To address this sensitivity, we suggest a specific role for specific (sub)models to counter unrealistic model outcomes. To support our proposal, we presented a selection of simulations for aggregated world regions, and showed how key results concerning the central variables can be subject to considerable change depending on the precise definitions of resource endowments and the technology-specificity of the factors.

Obviously, this also points towards future demand for IO-based modeling motivated by additional demands due to increased population, affluence, requirements of higher quality water, etc. Additionally, in the “real world”, if the price of the cleaner water is higher, typically the first type that is taken will be the cheaper one, (typically the lowest quality one). We argued that in order to represent this in the WTM/RCOT model we should present each of the options as “artificially” different technologies in which, even if all other inputs cost the same, the column is repeated, except for the factor input in question (the water quality type), which is technology specific. This allows choosing one or more technologies depending on the factor prices (for global cost minimizations). Hence, one of our recommendations is that ideally, we should represent as many columns as “equally possible” water quality inputs.

The conceptualizations and examples illustrate how understanding the different “water quality types”, “technologies and their water requirements” (implying mechanisms of technology specific/“mixed”/fully shared factors) and “water pricing” may have a very large effect on the interpretation of models and results regarding scarcity, constraints on factors, trade and virtual water trade, scarcity rents, dominant technologies of production and technological change in water intense sectors. Future work that can be derived from this way of thinking will be based on the exploration of extensive combinations of technologies and water factor frameworks with a large real-world database, thereby finding in depth results on specializations, scarcity, sensitivity to choices and so on.

We conclude then that the WTM/RCOT types of model are very relevant instruments for researchers studying water and their economic and policy implications, since knowing well (as we have tried to illustrate) which aspects are critical to defining good modeling and understanding the implications, provides a global comprehensive view of the water challenges in relation to other factors and economic drivers.

Further highly interesting questions can be derived from this type of results. The importance of the famous non-substitution theorem lies in the justification of the constancy of the coefficients of an input–output table, and it asserts: (i) that the choice of technique is independent of the patterns of final demand when efficiency prevails as to the use of a single primary factor, say labor; and (ii) that the commodity price vector is uniquely determined by the production structure, independently of final demand patterns. Translated into the notation and discussion here, the question then is if a shift in y (i.e., in final demand) might trigger a shift in technology in situations where more than one technology (per sector) is available. The answer was that it did not but that answer was given under very restrictive conditions, such as there being only one primary factor, labor, the wage being fixed (i.e., the elements of the π' vector in the WTM/RCOT literature), etc. The result (the non-substitution theorem) became famous because it was seen as strong support for Leontief’s assumption of fixed coefficients. However, the theorem has many aspects, many of which are important in judging its plausibility, empirical relevance, etc. For what we saw, there is a quite important logic in which (if a barrier is reached due to an increase in demand), less efficient technologies (with different production “recipe”) step in and the “first” factors get a rent. These could reveal that in practice increases in final demand may “induce” relevant shifts in technologies.

Supplementary Materials: The following are available online at <https://www.mdpi.com/2073-4411/13/4/459/s1>, Table S1: Baseline scenario A matrix (\$ of input per \$ unit of output of each technology in each region); Table S2: F matrix of the Baseline scenario; Table S3: f matrix of the Baseline scenario (million \$); Table S4: F matrix of the Water split H M L with more realistic coefficients (f1); Table S5: F matrix of the Water split H M L with more realistic coefficients with water returns (f2).

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